Optimum unambiguous discrimination of two mixed states and application to a class of similar states

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We study the measurement for the unambiguous discrimination of two mixed quantum states that are described by density operators ρ_1 and ρ_2 of rank d, the supports of which jointly span a $2d$-dimensional Hilbert space. Based on two conditions for the optimum measurement operators, and on a canonical representation for the density operators of the states, two equations are derived that allow the explicit construction of the optimum measurement, provided that the expression for the fidelity of the states has a specific simple form. For this case the problem is mathematically equivalent to distinguishing pairs of pure states, even when the density operators are not diagonal in the canonical representation. The equations are applied to the optimum unambiguous discrimination of two mixed states that are similar states, given by $\rho_2 = U\rho_1 U^\dagger$, and that belong to the class where the unitary operator U can be decomposed into multiple rotations in the d mutually orthogonal two-dimensional subspaces determined by the canonical representation.

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I. INTRODUCTION

The discrimination of nonorthogonal quantum states is of fundamental interest for many problems connected with quantum communication and quantum information and has consequently attracted a great deal of attention. An overwiew of the theoretical aspects of quantum state discrimination is given in recent review articles [1, 2]. The standard problem is the following: We assume that a quantum system is prepared in a certain state that is drawn with known prior probability from a finite set of known possible states, and we want to find the best measurement for determining the actual state of the system. When the given states are nonorthogonal, they cannot be discriminated perfectly, and therefore various measurement strategies have been developed that are optimized with respect to different criteria. The most prominent of these schemes are discrimination with minimum error [3] on the one hand, and optimum unambiguous discrimination [4, 5] on the other hand, and very recently also the strategy of discrimination with maximum confidence has been introduced [6].

In a measurement for unambiguous discrimination errors are not allowed, at the expense of admitting inconclusive results, where the measurement fails to give a definite answer. In this paper we restrict ourselves to considering only two given states that in the most general case are mixed states. Clearly, error-free discrimination of mixed states is only possible when the supports of the states are not identical. Note that the support of a quantum state is the Hilbert space spanned by those eigenvectors of its density operator that belong to nonzero eigenvalues, and the rank of a state is the dimension of its support. The optimum error-free measurement we are trying to find is the measurement that minimizes the average probability of getting an inconclusive result, or in other words, the average failure probability, where the prior probabilities for the occurrence of the different possible states are taken into account. We mention that recently unambiguous discrimination was also investigated without considering these prior probabilities, by requiring that in the best measurement the largest state-selective failure probability for any of the incoming states be as small as possible [7]. Here we stick to the traditional way of defining optimality for unambiguous discrimination by requiring that the average overall failure probability of the discriminating measurement be as small possible.

While the optimum measurement for the unambiguous discrimination of two pure states was found already a long time ago [4, 5], unambiguous discrimination involving mixed states, or sets of pure states, equivalently, became an object of research only more recently [8–20]. So far a general analytical solution for the optimum measurement that unambiguously distinguishes between two arbitrary mixed states does not exist yet, but a number of general results have been obtained. Several necessary and sufficient conditions for the optimum measurement have been derived [8, 9], and it has been shown that the solution can be found in an efficient way using the method of semi-definite programming [9]. Moreover, reduction theorems have been developed [10, 20] that can simplify the discrimination problems.

Lower bounds for the failure probability [11, 12, 19] as well as the conditions for saturating the bounds [13, 14, 19] have been also studied. It has been established that the minimum failure probability in the unambiguous strategy is at least twice as large as the minimum probability to get a wrong result when errors are allowed to occur [15]. As a consequence of the reduction theorems [8] it follows that the overall lower bound of the failure probability, proportional to the fidelity [11], can only be saturated when the dimension of the joint Hilbert space spanned by the supports of the two states is equal to the sum of their ranks. Even for this case the saturation of the bound depends sensitively on the structure of the

density operators and on their prior probabilities, and it is expected [18, 19] that in general the fidelity bound can be reached only in a very limited range of all parameters.

In a few special cases a complete analytical solution for the optimum measurement, valid for arbitrary prior probabilities of the two given states, has been derived. These cases are the unambiguous discrimination of
i) a pure state and an arbitrary mixed state, known as quantum state filtering [16, 17],
ii) two density operators of rank d in a $(d+1)$-dimensional joint Hilbert space [11], and
iii) two density operators of rank d that are simultaneously diagonal in the canonical basis [11] that separates the $2d$-dimensional joint Hilbert space into d mutually orthogonal two-dimensional subspaces [18].
The solution derived in Ref. [18] includes the unambiguous discrimination of two uniformly mixed states, which is equivalent to the discrimination of the two subspaces spanned by their supports. Moreover, the case iii) also applies to the comparison of two given pure states [21] having arbitrary prior probabilities [13, 22] and to the programmable discrimination [23] that distinguishes between two pure states when one [24] or both of them [23, 24, 25] are unknown and the discrimination is performed with the help of reference copies.

In the three cases listed above the optimum measurement can be constructed from the solutions for discriminating pairs of pure states. When such a reduction to pure-state discrimination problems is not possible, two classes of analytical solutions are known. First, general expressions for the optimum measurement operators have been derived which hold in the special case that for the given prior probabilities of the states the lower bound of the failure probability is saturated [14]. Second, the optimum measurement has been determined for two equally probable geometrically uniform states of rank two, described by density operators ρ_1 and ρ_2 with $\rho_2 = U\rho_1 U$, where $U^2 = I$ with I being the identity [20].

In the present paper we extend the above list of cases where a complete solution, valid for arbitrary prior probabilities of the states, can be obtained. We show that when a certain condition for the fidelity of the two states is fulfilled, the solution of the case iii) can be used to solve the optimization problem also for states that are not diagonal when represented with the help of the respective sets of orthonormal canonical basis states. In particular, the required condition for the fidelity is found to be satisfied for two mixed states that are similar, given by $\rho_2 = U\rho_1 U^\dagger$ where $U^\dagger U = I$, and that in addition belong to the class where the unitary operator U can be decomposed into multiple rotations in the two-dimensional subspaces determined by the canonical representation of the mixed states. Interestingly, by extending the quantum key distribution protocol based on two nonorthogonal pure states [26] to the case of two mixed states, it has been found a decade ago [27] that secure communication is only possible in this protocol when the two mixed states are connected by a rotation operator with a nonorthogonal angle and belong to the special class of states considered in this paper.

The paper is organized as follows: In Sec. II we review earlier results that are needed for the present investigation, and we derive our basic equations. The optimum measurement for the unambiguous discrimination of the special class of states considered in this paper is obtained in Sec. III, and the paper is concluded in Sec. IV.

II. GENERAL THEORY

A. Conditions for the lower bound of the failure probability

We start with a brief summary of the basic theoretical concepts and results that are needed for our further treatment. Any measurement for distinguishing two quantum states, characterized by the density operators ρ_1 and ρ_2, can be formally described by three positive detection operators obeying the equation

$$\Pi_0 + \Pi_1 + \Pi_2 = I, \tag{2.1}$$

where I is the identity. These detection operators are defined in such a way that $\mathrm{Tr}(\rho\Pi_{\rm k})$ with $k = 1, 2$ is the probability that a system prepared in a state ρ is inferred to be in the state ρ_k, while $\mathrm{Tr}(\rho\Pi_0)$ is the probability that the measurement fails to give a definite answer. The measurement is a von Neumann measurement when all detection operators are composed of projectors, otherwise it is a generalized measurement based on a positive operator-valued measure (POVM). From the detection operators Π_k schemes for realizing the measurement can be obtained using standard methods [28]. For the results of the measurement to be unambiguous, errors are not allowed to occur so that there is never a misidentification of any of the states. This leads to the requirement

$$\rho_1\Pi_2 = \rho_2\Pi_1 = 0 \tag{2.2}$$

[1, 2], which means that $\mathrm{Tr}(\rho_{\rm k}\Pi_0) = 1 - \mathrm{Tr}(\rho_{\rm k}\Pi_{\rm k})$ for $k = 1, 2$. When we denote the prior probabilities for the occurrence of the two states by η_1 and η_2, respectively, with $\eta_1 + \eta_2 = 1$, the total failure probability of the measurement, Q, is given by

$$\begin{aligned} Q &= \eta_1 \mathrm{Tr}(\rho_1\Pi_0) + \eta_2 \mathrm{Tr}(\rho_2\Pi_0) \\ &= 1 - \eta_1 \mathrm{Tr}(\rho_1\Pi_1) - \eta_2 \mathrm{Tr}(\rho_2\Pi_2). \end{aligned} \tag{2.3}$$

From the relation between the arithmetic and the geometric mean we get $Q \geq 2\sqrt{\eta_1\eta_2 \mathrm{Tr}(\rho_1\Pi_0)\mathrm{Tr}(\rho_2\Pi_0)}$, and because of the Cauchy-Schwarz-inequality this yields $Q \geq 2\sqrt{\eta_1\eta_2}\,\mathrm{Max}_V\,|\mathrm{Tr}(V\sqrt{\rho_1}\Pi_0\sqrt{\rho_2})|$ [12], where V describes an arbitrary unitary transformation. The failure probability takes its absolute minimum when the equality signs hold in these two relations, which is true if and only if both the equations

$$\eta_1 \mathrm{Tr}(\rho_1\Pi_0) = \eta_2 \mathrm{Tr}(\rho_2\Pi_0) \tag{2.4}$$

and $V\sqrt{\rho_1}\sqrt{\Pi_0} \sim \sqrt{\rho_2}\sqrt{\Pi_0}$ are fulfilled. After multiplying the second relation with its Hermitean conjugate, the two conditions for equality can be combined to yield [13]

$$\eta_1\sqrt{\Pi_0}\rho_1\sqrt{\Pi_0} = \eta_2\sqrt{\Pi_0}\rho_2\sqrt{\Pi_0}. \tag{2.5}$$

Substituting $\Pi_0 = I - \Pi_1 - \Pi_2$ into the inequality for the failure probability Q, given above, we arrive at

$$Q \geq 2\sqrt{\eta_1\eta_2}\, F(\rho_1, \rho_2), \tag{2.6}$$

where

$$F = \mathrm{Tr}\,[(\sqrt{\rho_2}\,\rho_1\sqrt{\rho_2})^{1/2}] = \mathrm{Tr}|\sqrt{\rho_1}\sqrt{\rho_2}| \tag{2.7}$$

is the fidelity [29]. From Eqs. (2.3) and (2.4) we conclude that the lower bound of the failure probability, proportional to the fidelity of the states, is obtained if and only if $\eta_1\mathrm{Tr}(\rho_1\Pi_0) = \eta_2\mathrm{Tr}(\rho_2\Pi_0) = \sqrt{\eta_1\eta_2}\,F$. This is equivalent to the two conditions [13]

$$\mathrm{Tr}(\rho_1\Pi_1) - 1 + \sqrt{\frac{\eta_2}{\eta_1}}\,F(\rho_1,\rho_2) \;=\; 0, \tag{2.8}$$

$$\mathrm{Tr}(\rho_2\Pi_2) - 1 + \sqrt{\frac{\eta_1}{\eta_2}}\,F(\rho_1,\rho_2) \;=\; 0 \tag{2.9}$$

that are the basic equations for our further treatment. Whenever we can find detection operators Π_1 and Π_2 satisfying Eqs. (2.8) and (2.9) while $\Pi_0 = I - \Pi_1 - \Pi_2$ is also a detection operator, i. e. a positive operator with eigenvalues between 0 and 1, then we are sure that these operators determine the optimum measurement for unambiguously discriminating the states, since they yield the lower bound of the failure probability, proportional to the fidelity. In the optimum measurement the lower bound can only be achieved when the necessary, but not sufficient, condition [13]

$$\frac{\mathrm{Tr}(P_2\rho_1)}{F} \leq \sqrt{\frac{\eta_2}{\eta_1}} \leq \frac{F}{\mathrm{Tr}(P_1\rho_2)} \tag{2.10}$$

is fulfilled, where the operators P_1 and P_2 are the projectors onto the supports of ρ_1 and ρ_2, respectively. It has been pointed out that there exist mixed states for which the fidelity bound cannot be reached for any value of the prior probabilities [13, 18].

B. The canonical representation of the density operators

When we want to explicitly determine the optimum detection operators, it is crucial to use convenient basis vectors for representing the two given states. From now on we focus our interest to the problem of distinguishing two states of rank d the supports of which jointly span a $2d$-dimensional Hilbert space, because it has been shown that the unambiguous discrimination of two arbitrary states can be reduced to this standard problem [10]. We start from the spectral representations for the two given states,

$$\rho_1 = \sum_{i=1}^{d} \tilde{r}_i|\tilde{r}_i\rangle\langle\tilde{r}_i|, \qquad \rho_2 = \sum_{i=1}^{d} \tilde{s}_i|\tilde{s}_i\rangle\langle\tilde{s}_i|. \tag{2.11}$$

The projectors onto the supports of the states then read

$$P_1 = \sum_{i=1}^{d} |\tilde{r}_i\rangle\langle\tilde{r}_i|, \qquad P_2 = \sum_{i=1}^{d} |\tilde{s}_i\rangle\langle\tilde{s}_i|. \tag{2.12}$$

As will become obvious later, for our purposes it is advantageous to perform two separate unitary basis transformations in the two Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ spanned by the supports of ρ_1 and ρ_2, respectively, yielding two new sets of orthonormal basis states that are denoted by $\{|r_i\rangle\}$ and $\{|s_i\rangle\}$ and have the property that

$$\langle r_i|r_j\rangle \;=\; \langle s_i|s_j\rangle = \delta_{ij}, \tag{2.13}$$

$$\langle r_i|s_j\rangle \;=\; \langle s_j|r_i\rangle = C_i\delta_{ij}, \quad 0 \leq C_i \leq 1. \tag{2.14}$$

Basis states of this kind have been used already previously to study the unambiguous discrimination of two mixed states [11, 18] and to construct a very simple example [13]. After the basis transformations have been performed, the density operators take the form

$$\rho_1 = \sum_{i,j=1}^{d} r_{ij}|r_i\rangle\langle r_j|, \qquad \rho_2 = \sum_{i,j=1}^{d} s_{ij}|s_i\rangle\langle s_j|. \tag{2.15}$$

In the following we shall refer to Eqs. (2.15) together with Eqs. (2.13) and (2.14) as the canonical representation of the two given density operators.

In order to show that for any two density operators of rank d jointly spanning a $2d$-dimensional Hilbert space the canonical representation always exists, and to give also a recipe how it can be constructed, we rely on the treatment given in Ref. [27]. First we observe that the operator $P_1P_2P_1$ is Hermitean, and that its eigenstates, which we denote by $|r_i\rangle$, therefore span a complete d-dimensional orthonormal basis in $\mathcal{H}_1$. Because P_2 and P_1 are projectors, it follows that $\langle r_i|P_2^2|r_i\rangle = \langle r_i|P_1P_2P_1|r_i\rangle$. Clearly, the norm of the state $P_2|r_i\rangle$ is not larger than 1, and moreover it is non-zero since the joint Hilbert space spanned by the supports of the two density operators is assumed to be $2d$-dimensional. Hence we can establish the eigenvalue equation

$$P_1P_2P_1|r_i\rangle = P_1P_2|r_i\rangle = C_i^2|r_i\rangle, \tag{2.16}$$

where $0 < C_i \leq 1$ and $\langle r_i|r_j\rangle = \delta_{ij}$. Now we introduce the normalized states in $\mathcal{H}_2$ that are given by [27]

$$|s_j\rangle = \frac{1}{C_j}\,P_2|r_j\rangle = \frac{1}{C_j}\,P_2P_1|r_j\rangle \tag{2.17}$$

and obey the equations

$$\langle s_i|s_j\rangle \;=\; \frac{1}{C_iC_j}\,\langle r_i|P_1P_2P_1|r_j\rangle, \tag{2.18}$$

$$\langle r_i|s_j\rangle \;=\; \frac{1}{C_j}\,\langle r_i|P_1P_2P_1|r_j\rangle. \tag{2.19}$$

Taking into account that $\langle r_i|P_1P_2P_1|r_j\rangle = C_i^2\delta_{ij}$ because of Eq. (2.16), we immediately arrive at Eqs. (2.13) and (2.14). Thus we have shown that Eq. (2.16) together with Eq. (2.17) provides the means for determining the two sets of canonical basis states $\{|r_i\rangle\}$ and $\{|s_i\rangle\}$. Obviously, this requires the solution of a dth-order algebraic equation, resulting from the eigenvalue equation, Eq. (2.16). We still remark that by making use of $P_2|r_i\rangle = C_i|s_i\rangle$ and $P_1|s_i\rangle = C_i|r_i\rangle$, Eq. (2.16) can be transformed into $C_i^2\ P_2|r_i\rangle = P_2P_1P_2|r_i\rangle$ which, with the help of Eq. (2.17), leads to the alternative eigenvalue equation $P_2P_1|s_i\rangle = P_1P_2P_1|s_i\rangle = C_i^2|s_i\rangle$, as expected for symmetry reasons.

C. Construction of the optimum detection operators

Having obtained the canonical representation of the density operators to be discriminated, we are now in the position to make an explicit general Ansatz for the detection operators Π_1 and Π_2 that enable the unambiguous discrimination by satisfying Eq. (2.2). For this purpose we define the states

$$|v_i\rangle = \frac{|r_i\rangle - C_i|s_i\rangle}{S_i}, \quad |w_i\rangle = \frac{|s_i\rangle - C_i|r_i\rangle}{S_i}, \tag{2.20}$$

where $S_i = \sqrt{1-C_i^2}$. Making use of Eqs. (2.13) and (2.14) it follows that

$$\langle v_i|v_j\rangle = \langle w_i|w_j\rangle = \delta_{ij} \tag{2.21}$$

and, most importantly,

$$\langle v_i|s_j\rangle = \langle w_i|r_j\rangle = 0. \tag{2.22}$$

The two joint sets of states $\{\{|s_i\rangle\},\{|v_i\rangle\}\}$, on the one hand, and $\{\{|r_i\rangle\},\{|w_i\rangle\}\}$, on the other hand, form two different complete orthonormal basis systems in our $2d$-dimensional Hilbert space. Their mutual geometrical orientation is characterized by the relations

$$\langle v_i|r_j\rangle = \langle w_i|s_j\rangle = S_i\delta_{ij}, \tag{2.23}$$

in addition to $\langle v_i|w_j\rangle = -C_i\,\delta_{ij} = -\langle r_i|s_j\rangle$. In accordance with our earlier work [13] we can now make the general Ansatz

$$\Pi_1 = \sum_{i,j=1}^{d} \alpha_{ij}|v_i\rangle\langle v_j|, \quad \Pi_2 = \sum_{i,j=1}^{d} \beta_{ij}|w_i\rangle\langle w_j| \tag{2.24}$$

which because of Eqs. (2.15) and (2.22) guarantees that $\rho_1\Pi_2 = \rho_2\Pi_1 = 0$, as required for unambiguous discrimination. For these operators to describe a physical measurement, the coefficients α_{ij} and β_{ij} must be chosen in such a way that their eigenvalues, as well as the eigenvalues of Π_0, are nonnegative and not larger than 1. Using the expression $\Pi_1 = \sum_{i,j}\alpha_{ij}I|v_i\rangle\langle v_j|I$, where

$$I = \sum_{i=1}^{d}(|r_i\rangle\langle r_i| + |w_i\rangle\langle w_i|) \tag{2.25}$$

is the unity operator in the $2d$-dimensional Hilbert space, we can represent the operator $\Pi_0 = I - \Pi_1 - \Pi_2$ in the form

$$\Pi_0 = \sum_{i,j=1}^{d}[(\delta_{ij} - \alpha_{ij}S_iS_j)|r_i\rangle\langle r_j| + \alpha_{ij}S_iC_j|r_i\rangle\langle w_j| + \alpha_{ji}S_jC_i|w_i\rangle\langle r_j| + (\delta_{ij} - \alpha_{ij}C_iC_j - \beta_{ij})|w_i\rangle\langle w_j|]. \tag{2.26}$$

Moreover, from Eqs. (2.24) and (2.3) we obtain an explicit expression for the failure probability, given by

$$Q = 1 - \sum_{i,j=1}^{d} S_iS_j(\eta_1\alpha_{ij}r_{ji} + \eta_2\beta_{ij}s_{ji}). \tag{2.27}$$

For brevity, in the rest of the paper we denote the diagonal elements of the density operators and of the detection operators as

$$r_{ii} \equiv r_i, \quad s_{ii} \equiv s_i, \quad \alpha_{ii} \equiv \alpha_i, \quad \beta_{ii} \equiv \beta_i. \tag{2.28}$$

Since $\sum_i r_i = \sum_i s_i = 1$, the conditions for the achievement of the absolute minimum of the failure probability, Eqs. (2.8) and (2.9), can be rewritten as

$$\sum_{i,j=1}^{d}(S_iS_j\alpha_{ij} - \delta_{ij})r_{ji} + \sqrt{\frac{\eta_2}{\eta_1}}F(\{C_i, r_{ij}, s_{ij}\}) = 0, \tag{2.29}$$

$$\sum_{i,j=1}^{d}(S_iS_j\beta_{ij} - \delta_{ij})s_{ji} + \sqrt{\frac{\eta_1}{\eta_2}}F(\{C_i, r_{ij}, s_{ij}\}) = 0, \tag{2.30}$$

where the fidelity depends on the parameters that characterize the density operators in the canonical representation, given by Eqs. (2.13)-(2.15). Clearly, in general the coefficients α_{ij} and β_{ij} are not uniquely determined by these two equations alone, and a complete system of equations would have to be found, taking into account Eq. (2.5). However, under certain conditions Eqs. (2.29) and (2.30) are sufficient for obtaining the optimum measurement, as we shall see in the following. In particular, this is the case when the canonical representation of the density operators is such that the expression for the fidelity has a specific form, depending only on the diagonal elements r_i and s_i.

D. An analytical solution for the optimum measurement

We start by reconsidering a problem that has been recently explicitly solved with the help of a slightly different approach [18]. We assume that the density operators are diagonal in the canonical representation, i. e.

$$\rho_1 = \sum_{i=1}^{d} r_i|r_i\rangle\langle r_i|, \qquad \rho_2 = \sum_{i=1}^{d} s_i|s_i\rangle\langle s_i|, \tag{2.31}$$

where Eqs. (2.13) and (2.14) hold for the eigenstates of the density operators. The fidelity is then readily calculated from Eq. (2.7) as

$$F = \sum_{i=1}^{d} C_i \sqrt{r_i s_i}, \tag{2.32}$$

and Eqs. (2.29) and (2.30) take the form

$$\sum_{i=1}^{d} \left(S_i^2 \alpha_i - 1 + \sqrt{\frac{\eta_2 s_i}{\eta_1 r_i}} C_i \right) r_i \;=\; 0, \tag{2.33}$$

$$\sum_{i=1}^{d} \left(S_i^2 \beta_i - 1 + \sqrt{\frac{\eta_1 r_i}{\eta_2 s_i}} C_i \right) s_i \;=\; 0. \tag{2.34}$$

A solution for the diagonal elements of the optimum detection operators can now be immediately read out. It is given by $\alpha_i = \alpha_i^{\rm o}$ and $\beta_i = \beta_i^{\rm o}$, where

$$\alpha_i^{\rm o} = \frac{1}{S_i^2}\left(1 - \sqrt{\frac{\eta_2 s_i}{\eta_1 r_i}} C_i\right), \quad \beta_i^{\rm o} = \frac{1}{S_i^2}\left(1 - \sqrt{\frac{\eta_1 r_i}{\eta_2 s_i}} C_i\right). \tag{2.35}$$

According to Eq. (2.27) the failure probability Q does not depend on the nondiagonal elements of the detection operators when $r_{ij} = r_i\delta_{ij}$ and $s_{ij} = s_i\delta_{ij}$. We therefore conclude that in the optimum measurement

$$\alpha_{ij} = \alpha_i \delta_{ij}, \quad \beta_{ij} = \beta_i \delta_{ij}, \tag{2.36}$$

since this requirement guarantees that α_i and β_i can be made as large as possible while Π_0 is still a positive operator, i. e. that the failure probability becomes as small as possible. Because of the condition on the eigenvalues of the detection operators we have to require that $0 \le \alpha_i^{\rm o}, \beta_i^{\rm o} \le 1$. Therefore Eqs. (2.35) only represent a physical solution for the optimum measurement when the ratio η_2/η_1 falls within certain intervals. After replacing the coefficients $\alpha_i^{\rm o}$ and $\beta_i^{\rm o}$ outside these intervals by their values at the boundaries, in order to make Q as small as possible, we arrive at

$$\begin{aligned}
&\alpha_i^{\rm opt} = 1, \quad \beta_i^{\rm opt} = 0 \quad && \text{if} \quad \sqrt{\tfrac{\eta_2}{\eta_1}} \le C_i \sqrt{\tfrac{r_i}{s_i}}, \\
&\alpha_i^{\rm opt} = \alpha_i^{\rm o}, \quad \beta_i^{\rm opt} = \beta_i^{\rm o} \quad && \text{if} \quad C_i\sqrt{\tfrac{r_i}{s_i}} \le \sqrt{\tfrac{\eta_2}{\eta_1}} \le \tfrac{1}{C_i}\sqrt{\tfrac{r_i}{s_i}}, \\
&\alpha_i^{\rm opt} = 0, \quad \beta_i^{\rm opt} = 1 \quad && \text{if} \quad \tfrac{1}{C_i}\sqrt{\tfrac{r_i}{s_i}} \le \sqrt{\tfrac{\eta_2}{\eta_1}},
\end{aligned} \tag{2.37}$$

in accordance with Ref. [18]. The optimum detection operators are then given by

$$\Pi_1^{\rm opt} = \sum_{i=1}^{d} \alpha_i^{\rm opt} |v_i\rangle\langle v_i|, \quad \Pi_2^{\rm opt} = \sum_{i=1}^{d} \beta_i^{\rm opt} |w_i\rangle\langle w_i|, \tag{2.38}$$

and

$$\begin{aligned}
\Pi_0^{\rm opt} = \sum_{i=1}^{d} &[(1 - \alpha_i^{\rm opt} S_i^2)|r_i\rangle\langle r_i| + \alpha_i^{\rm opt} S_i C_i |r_i\rangle\langle w_i| \\
&+ \alpha_i^{\rm opt} S_i C_i |w_i\rangle\langle r_i| + (1 - \alpha_i^{\rm opt} C_i^2 - \beta_i^{\rm opt})|w_i\rangle\langle w_i|],
\end{aligned} \tag{2.39}$$

where in the latter expression Eqs. (2.26) and (2.36) have been used. In order to show that these operators indeed describe a physical measurement, we still have to verify that Π_0 is a positive operator. From Eq. (2.39) it becomes obvious that Π_0 can be represented by a matrix which consists of d decoupled two by two matrices. Taking into account that $S_i^2 \alpha_i^o \beta_i^o = \alpha_i^o + \beta_i^o$, we find after minor algebra that for each of these matrices one eigenvalue is zero and the other is given by

$$\lambda_i = \alpha_i^o + \beta_i^o \qquad \text{if} \quad C_i\sqrt{\tfrac{r_i}{s_i}} \le \sqrt{\tfrac{\eta_2}{\eta_1}} \le \tfrac{1}{C_i}\sqrt{\tfrac{r_i}{s_i}}, \tag{2.40}$$

or by $\lambda_i = 1$ otherwise [18]. It is easy to check that the condition $0 \le \lambda_i \le 1$ is indeed fulfilled for the eigenvalues λ_i of the operator Π_0.

A few direct conclusions can be drawn from the Eqs. (2.37). Obviously, when for the given prior probabilities of the two mixed states there does not exist a single value of i for which the condition in the middle line of Eq. (2.37) is fulfilled, then the optimum measurement is a von Neumann measurement, where the detection operators are projectors. In this case the failure probability of the optimum measurement is given by

$$\begin{aligned}
Q_{\rm opt} &= 1 - \eta_1 \textstyle\sum_{i=1}^{d} S_i^2 r_i \quad \text{if} \quad \sqrt{\tfrac{\eta_2}{\eta_1}} \le {\rm Min}_i \left\{ C_i\sqrt{\tfrac{r_i}{s_i}} \right\}, \\
Q_{\rm opt} &= 1 - \eta_2 \textstyle\sum_{i=1}^{d} S_i^2 s_i \quad \text{if} \quad \sqrt{\tfrac{\eta_2}{\eta_1}} \ge {\rm Max}_i \left\{ \tfrac{1}{C_i}\sqrt{\tfrac{r_i}{s_i}} \right\}.
\end{aligned} \tag{2.41}$$

In all other cases the optimum measurement is a generalized measurement, but only when the condition in the middle line of Eq. (2.37) is fulfilled for each single value of i, $(i = 1, \ldots, d)$, the fidelity bound of the failure probability is obtained. Thus we have that $Q_{\rm opt} = 2\sqrt{\eta_1\eta_2}F$ if

$${\rm Max}_i \left\{ C_i\sqrt{\tfrac{r_i}{s_i}} \right\} \le \sqrt{\tfrac{\eta_2}{\eta_1}} \le {\rm Min}_i \left\{ \tfrac{1}{C_i}\sqrt{\tfrac{r_i}{s_i}} \right\}. \tag{2.42}$$

Clearly, when ${\rm Max}_i \left\{ C_i\sqrt{\tfrac{r_i}{s_i}} \right\} \ge {\rm Min}_i \left\{ \tfrac{1}{C_i}\sqrt{\tfrac{r_i}{s_i}} \right\}$ the condition given by Eq. (2.42) can never hold true and the overall lower bound of the failure probability cannot be reached.

It is important to observe that the solution expressed by Eqs. (2.36) and (2.37) holds whenever the fidelity takes the form given by Eq. (2.32), since due to Eq. (2.36) the nondiagonal density matrix elements r_{ij} and s_{ij} do not enter the Eqs. (2.29) and (2.30). In Sec. III we apply this solution to the optimum unambiguous discrimination of two particular density operators that do not have to be diagonal in the canonical representation.

III. DISCRIMINATION OF STATES BELONGING TO A CLASS OF SIMILAR STATES

A. The canonical representation and the fidelity

Now we turn our attention to the unambiguous discrimination of two mixed states ρ_1 and ρ_2 of rank d

that are connected via a unitary transformation in the $2d$-dimensional Hilbert space spanned by their joint supports,

$$\rho_2 = U\ \rho_1\ U^\dagger, \tag{3.1}$$

where $U^\dagger = U^{-1}$. Since we want to determine the optimum measurement by means of applying Eqs. (2.29) and (2.30), we first have to express the condition on the states within the framework of the canonical representation. By inserting the respective density operators, given by Eqs. (2.15), into Eq. (3.1), we obtain

$$\rho_2 = \sum_{i,j=1}^{d} s_{ij}|s_i\rangle\langle s_j| = \sum_{i,j=1}^{d} r_{ij} U|r_i\rangle\langle r_j|U^\dagger, \tag{3.2}$$

where $\langle r_i|s_j\rangle = C_i\delta_{ij}$ and $\langle s_i|s_j\rangle = \langle r_i|r_j\rangle = \delta_{ij}$. The operator U transforms any state in the support of ρ_1 into a state in the support of ρ_2 which means in particular that $U|r_i\rangle = \sum_k c_{ik}|s_k\rangle$, where $\sum_k c_{ik}c^*_{jk} = \langle r_i|r_j\rangle = \delta_{ij}$. In general, the calculation of the fidelity of these two mixed states is a difficult problem and cannot be performed analytically. In the following we therefore restrict ourselves to a special class of unitary transformations.

We assume that the unitary transformation U can be decomposed into d independent unitary transformations U_i that act in the d mutually orthogonal two-dimensional subspaces spanned by the pairs of nonorthogonal states $|r_i\rangle$ and $|s_i\rangle$. In each of the subspaces a particular orthonormal basis is given by the states $|r_i\rangle$ and $|w_i\rangle$, where

$$|w_i\rangle = \frac{1}{S_i}\left(|s_i\rangle - C_i|r_i\rangle\right). \tag{3.3}$$

Since according to Eqs. (2.13) and (2.14) the inner products of any two states in the combined set of the basis states of the two density operators are real, the class of transformations we consider is described by [27]

$$U = U_1(\theta_1)\otimes U_2(\theta_2)\otimes\ldots\otimes U_d(\theta_d), \tag{3.4}$$

where the transformations in the subspaces are rotations by the angle θ_i,

$$U_i(\theta_i) = \exp\left[\,\theta_i\left(|w_i\rangle\langle r_i| - |r_i\rangle\langle w_i|\right)\right]. \tag{3.5}$$

As can be verified by expanding $U_i(\theta_i)$ in terms of powers of θ_i, this is equivalent to

$$U_i(\theta_i)|r_j\rangle = \begin{cases} \cos\theta_i|r_i\rangle + \sin\theta_i|w_i\rangle & \text{if } i=j \\ |r_j\rangle & \text{if } i\neq j. \end{cases} \tag{3.6}$$

In order to obtain the canonical representation of the density operators, we have to determine the eigenvalues and eigenstates of the operator $P_1P_2P_1$, see Eq. (2.16). The projectors onto the supports of ρ_1 and ρ_2 read

$$P_1 = \sum_{i=1}^{d}|r_i\rangle\langle r_i|, \quad P_2 = \sum_{i=1}^{d}U|r_i\rangle\langle r_i|U^\dagger, \tag{3.7}$$

where the expression for P_2 follows from the right-hand side of Eq. (3.2). By applying Eq. (3.6) we easily find that

$$P_1P_2P_1 = \sum_{i=1}^{d}\cos^2\theta_i|r_i\rangle\langle r_i|, \tag{3.8}$$

and Eq. (2.16) therefore immediately yields

$$C_i = \cos\theta_i. \tag{3.9}$$

From Eqs. (3.6) and Eq. (3.3) we then obtain

$$U|r_i\rangle = |s_i\rangle \tag{3.10}$$

which means that

$$\langle r_j|U|r_i\rangle \ = \ C_i\delta_{ij}. \tag{3.11}$$

After calculating the matrix element $\langle r_i|\rho_2|r_j\rangle$ from both expressions in Eq. (3.2), using Eq. (3.11), we finally get

$$s_{ij} = r_{ij}. \tag{3.12}$$

Hence under the condition given by Eq. (3.4) our starting equation, Eq . (3.2), can only be fulfilled when

$$\rho_1 = \sum_{i,j=1}^{d} r_{ij}|r_i\rangle\langle r_j|, \quad \rho_2 = \sum_{i,j=1}^{d} r_{ij}|s_i\rangle\langle s_j|. \tag{3.13}$$

In other words, the two mixed states we consider differ by the orientation of their respective canonical basis states in the $2d$-dimensional Hilbert space, but the relative weights of these states and the coherences between them are the same.

After having specified the relation between the matrix elements of the two density operators, our next step before applying Eqs. (2.29) and (2.30) is the calculation of the fidelity. From Eq. (3.1) we obtain $\sqrt{\rho_2} = U\sqrt{\rho_1}U^\dagger$ and Eq. (2.7) therefore yields

$$\begin{aligned} F \ &= \ \mathrm{Tr}|\sqrt{\rho_1}U\sqrt{\rho_1}U^\dagger| \\ &= \ \mathrm{Tr}[(\sqrt{\rho_1}U\sqrt{\rho_1}U^\dagger\ U\sqrt{\rho_1}U^\dagger\sqrt{\rho_1})^{\frac{1}{2}}] \\ &= \ \mathrm{Tr}|\sqrt{\rho_1}U\sqrt{\rho_1}|, \end{aligned} \tag{3.14}$$

where we made use of the fact that $U^\dagger U = I$. Writing the unity operator in our $2d$-dimensional Hilbert space as $I = \sum_{i=1}^{d}(|r_i\rangle\langle r_i| + |w_i\rangle\langle w_i|)$ and inserting it twice, taking into account that $\rho_1|w_i\rangle = 0$, we obtain

$$\begin{aligned} F \ &= \ \mathrm{Tr}|\sqrt{\rho_1}\sum_{i,j}|r_i\rangle\langle r_i|U|r_j\rangle\langle r_j|\sqrt{\rho_1}| \\ &= \ \mathrm{Tr}|\sum_{i}C_i\sqrt{\rho_1}|r_i\rangle\langle r_i|\sqrt{\rho_1}|, \end{aligned} \tag{3.15}$$

where Eq. (3.11) has been used. Defining the vector $|a_i\rangle = \sqrt{\rho_1}|r_i\rangle$, we find that $F = \sum_i C_i\mathrm{Tr}(|a_i\rangle\langle a_i|)$ and arrive at the final result

$$F = \sum_{i=1}^{d}C_i\langle r_i|\rho_1|r_i\rangle = \sum_{i=1}^{d}C_ir_i. \tag{3.16}$$

Interestingly, for the class of states we consider the fidelity does not depend on the nondiagonal elements of the density operators in the canonical representation, no matter what is the kind of the individual unitary transformations in the two-dimensional subspaces.

B. The optimum measurement

We are now prepared to determine the measurement for the optimum unambiguous discrimination. Upon inserting the expression for the fidelity, Eq. (3.16), into our basic conditions, Eqs. (2.29) and (2.30), taking into account that $s_{ij} = r_{ij}$, we arrive at the two equations

$$\begin{aligned} \sum_{i\neq j} S_i S_j \alpha_{ij} r_{ji} + \sum_i \left(S_i^2 \alpha_i - 1 + \sqrt{\frac{\eta_2}{\eta_1}} C_i \right) r_i &= 0, \\ \sum_{i\neq j} S_i S_j \beta_{ij} r_{ji} + \sum_i \left(S_i^2 \beta_i - 1 + \sqrt{\frac{\eta_1}{\eta_2}} C_i \right) r_i &= 0 \end{aligned} \tag{3.17}$$

that have to be fulfilled by the coefficients determining the optimum detection operators. Because of the special structure of these equations, resulting from the specific expression for the fidelity, we are free to make the Ansatz

$$\alpha_{ij} = \alpha_i \delta_{ij}, \quad \beta_{ij} = \beta_i \delta_{ij}. \tag{3.18}$$

Obviously, the problem to be solved is then reduced to the problem expressed by Eqs. (2.33) and (2.34), in the special case that $r_i = s_i$. The previous solution, given by Eqs. (2.35) - (2.37), therefore can be immediately applied and the optimum coefficients read

$$\begin{array}{lll} \alpha_i^{\rm opt} = 1, \quad \beta_i^{\rm opt} = 0 & \text{if} & \sqrt{\frac{\eta_2}{\eta_1}} \leq C_i, \\ \alpha_i^{\rm opt} = \alpha_i^{\rm o}, \quad \beta_i^{\rm opt} = \beta_i^{\rm o} & \text{if} & C_i \leq \sqrt{\frac{\eta_2}{\eta_1}} \leq \frac{1}{C_i}, \\ \alpha_i^{\rm opt} = 0, \quad \beta_i^{\rm opt} = 1 & \text{if} & \frac{1}{C_i} \leq \sqrt{\frac{\eta_2}{\eta_1}}, \end{array} \tag{3.19}$$

where

$$\alpha_i^{\rm o} = \frac{1}{S_i^2}\left(1 - \sqrt{\frac{\eta_2}{\eta_1}} C_i\right), \quad \beta_i^{\rm o} = \frac{1}{S_i^2}\left(1 - \sqrt{\frac{\eta_1}{\eta_2}} C_i\right). \tag{3.20}$$

The solutions for the optimum detection operators follow by inserting the optimum coefficients into Eqs. (2.38) and (2.39).

In order to obtain compact results for the minimum failure probability, $Q_{\rm opt}$, ensuing from the optimum measurement, it will be useful to adopt the convention that

$$C_1 \leq C_2 \leq \ldots \leq C_{d-1} \leq C_d. \tag{3.21}$$

After inserting Eqs. (3.18) - (3.20) into the equation for the failure probability Q, Eq. (2.27), taking into account that $r_i = s_i$, we find again that the structure of the resulting expressions depends on the ratio of the prior probabilities. If the latter is such that one of the two von Neumann measurements is optimal, the minimum failure probability takes the form

$$\begin{array}{lll} Q_{\rm opt} = 1 - \eta_1 \sum_{i=1}^d S_i^2 r_i & \text{if} & \sqrt{\frac{\eta_2}{\eta_1}} \leq C_1, \\ Q_{\rm opt} = 1 - \eta_2 \sum_{i=1}^d S_i^2 r_i & \text{if} & \sqrt{\frac{\eta_2}{\eta_1}} \geq \frac{1}{C_1}. \end{array} \tag{3.22}$$

On the other hand, with respect to the saturation of the fidelity bound we find that

$$Q_{\rm opt} = 2\sqrt{\eta_1\eta_2} F \qquad \text{if} \quad C_d \leq \sqrt{\frac{\eta_2}{\eta_1}} \leq \frac{1}{C_d}, \tag{3.23}$$

where $F = \sum_{i=1}^d C_i r_i$. In the intermediate regions of the ratio of the prior probabilities the optimum failure probability can be written as

$$Q_{\rm opt} = 1 - \sum_{i=1}^k (1 - 2\sqrt{\eta_1\eta_2} C_i) r_i - \eta_1 \sum_{i=k+1}^d S_i^2 r_i \tag{3.24}$$
$$\text{if} \quad C_k \leq \sqrt{\frac{\eta_2}{\eta_1}} \leq C_{k+1} \quad (1 \leq k \leq d-1)$$

and

$$Q_{\rm opt} = 1 - \sum_{i=1}^k (1 - 2\sqrt{\eta_1\eta_2} C_i) r_i - \eta_2 \sum_{i=k+1}^d S_i^2 r_i \tag{3.25}$$
$$\text{if} \quad \frac{1}{C_{k+1}} \leq \sqrt{\frac{\eta_2}{\eta_1}} \leq \frac{1}{C_k} \quad (1 \leq k \leq d-1).$$

Clearly, in dependence on the ratio of the prior probabilities of the states, there are in general $2d+1$ parameter regions in which the optimum measurement operators have a different structure and consequently the expression for the optimum failure probability takes a different form. These regions do not depend on the matrix elements of the density operators, but only on the canonical angles, that is on the constants C_i. For $d = 2$, the calculation of C_1 and C_2 can be easily performed analytically by means of Eq. (2.16) since it only amounts to the solution of a quadratic equation.

It is interesting to compare the parameter interval in which the fidelity bound of the failure probability can be actually achieved, specified in Eq. (3.23), with the respective parameter interval following from a necessary, but not sufficient condition [13], as given in Eq. (2.10). Representing P_1 and P_2 as $\sum_{i=1}^d |r_i\rangle\langle r_i|$ and $\sum_{i=1}^d |s_i\rangle\langle s_i|$, respectively, we find that $\mathrm{Tr}(P_2\rho_1) = \mathrm{Tr}(P_2\rho_1) = \sum_{i=1}^d C_i^2 r_i$. The former interval is necessarily not larger than the latter, the relative difference between the intervals obviously being characterized by the ratio $\sum_{i=1}^d C_i^2 r_i / \sum_{i=1}^d C_i C_d r_i$, where the explicit expression for the fidelity has been taken into account.

Two special cases are worth mentioning. In the first one the two mixed states have equal prior probabilities to occur, $\eta_1 = \eta_2 = 0.5$. Since the inequality $C_d \leq 1 \leq 1/C_d$ certainly holds for any $C_d = \cos\theta_d \leq 1$, it becomes obvious from Eq. (3.23) that in this case the fidelity bound of the failure probability can always be reached.

The second special case refers to identical canonical angles, $C_i = \cos\theta$ for $i = 1, \dots, d$ which means that the two density operators are connected via a rotation by the angle θ. We mention that for a nonorthogonal angle θ this is exactly the condition that has been derived in Ref. [27] as the prerequisite for secure quantum communication when the two-pure-state protocol [26] is extended to two mixed states. In this case it follows that $\mathrm{Tr}(P_1\rho_2) = \mathrm{Tr}(P_2\rho_1) = F^2 = \cos^2\theta$ and our general solution, represented by Eqs. (3.22) - (3.25) reduces to

$$Q_{\rm opt} = \begin{cases} 2\sqrt{\eta_1\eta_2}F & \text{if } F \le \sqrt{\frac{\eta_1}{\eta_2}} \le \frac{1}{F} \\ \eta_{\rm min} + \eta_{\rm max}F^2 & \text{otherwise,} \end{cases} \tag{3.26}$$

where $\eta_{\rm min}(\eta_{\rm max})$ denotes the smaller (larger) of the prior probabilities. This result exactly corresponds to the solution for the optimum unambiguous discrimination of two pure states [5].

IV. CONCLUSIONS

In this paper we have shown that an analytical solution for the optimum unambiguous discrimination of two mixed states can be obtained provided that the expression for their fidelity is given by Eq. (2.32), where the density operators are represented with the help of the canonical basis that separates the joint Hilbert space into d mutually orthogonal two-dimensional subspaces. The discrimination problem is then mathematically equivalent to distinguishing pairs of pure states. We applied the solution to the discrimination of two mixed states that belong to a special class of similar states. The density operators of these states do not have to be diagonal in the canonical representation. Our results might be also of interest for quantum cryptography, where states of the kind considered in this paper play a role [27].

We still note that after finishing this work a related paper appeared [19] where the authors investigate lower bounds of the failure probability by introducing a different kind of state vectors spanning the joint Hilbert space. These states are defined by the requirement that for any two density operators the expression for the fidelity is of a form equivalent to Eq. (2.32). In contrast to the canonical basis states considered in the present paper, the states introduced in [19] do not necessarily provide an orthogonal basis in the supports of the two density operators.

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